World Academy of Science, Engineering and Technology International Journal of Computer and Information Engineering Vol:18, No:01, 2024

AutoML: Comprehensive Review and Application to Engineering Datasets

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Abstract: The development of accurate machine learning and deep learning models traditionally demands hands-on expertise and a solid background to fine-tune hyperparameters. With the continuous expansion of datasets in various scientific and engineering domains, researchers increasingly turn to machine learning methods to unveil hidden insights that may elude classic regression techniques. This surge in adoption raises concerns about the adequacy of the resultant meta-models and, consequently, the interpretation of the findings. In response to these challenges, automated machine learning (AutoML) emerges as a promising solution, aiming to construct machine learning models with minimal intervention or guidance from human experts. AutoML encompasses crucial stages such as data preparation, feature engineering, hyperparameter optimization, and neural architecture search. This paper provides a comprehensive overview of the principles underpinning AutoML, surveying several widely-used AutoML platforms. Additionally, the paper offers a glimpse into the application of AutoML on various engineering datasets. By comparing these results with those obtained through classical machine learning methods, the paper quantifies the uncertainties inherent in the application of a single ML model versus the holistic approach provided by AutoML. These examples showcase the efficacy of AutoML in extracting meaningful patterns and insights, emphasizing its potential to revolutionize the way we approach and analyze complex datasets.

Keywords: automated machine learning, uncertainty, engineering dataset, regression

Conference Title: ICMLC 2024: International Conference on Machine Learning and Cybernetics

Conference Location: Istanbul, Türkiye Conference Dates: January 29-30, 2024